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Long-range electron-hole exchange in semiconductor quantum dots

Seungwon Lee, Lars Jönsson, John W. Wilkins, Garnett W. Bryant, and Gerhard Klimeck

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Abstract: In contrast to the local exchange interaction in bulk material, the electron-hole exchange in semiconductor quantum dots can have a large long-range component. This long-range exchange arises from the local (onsite) nonorthogonality of the electron and hole wave functions. Consequently, the exchange charge density has a monopole moment that necessarily leads to Coulomb exchange integrals with integrands extending over the whole dot. Using empirical tight-binding wave functions, we describe explicitly the structure of the long-range exchange for spherical Si, InAs, and CdSe dots. For direct-gap InAs and CdSe, pairs of electron and hole wave functions that exhibit a large long-range exchange have no local orthogonality, but have only a global orthogonality --- for example, a 2s- or p-like distribution of the exchange-charge density over the whole dot. For indirect-gap Si, the local orthogonality is recovered in a few lattice constants, about 15\ \ regardless of dot size, due to the overall phase difference between the electron and hole wave functions in an indirect material.

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